1,5,7-Trimethyl-2-nitro-imidazo[4,5,d]pyrimidin-4,6

Inchi: InChI=1S/C8H9N5O4/c1-10-5-4(9-7(10)13(16)17)6(14)12(3)8(15)11(5)2/h1-3H3
InchiKey: BYTUYCJYACKIDG-UHFFFAOYSA-N
Formula: C8H9N5O4
SMILES: Cn1c(=O)c2nc([N+](=O)[O-])n(C)c2n(C)c1=O
Mol. weight [g/mol]: 239.19
CAS: 153285-56-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.40		Crippen Method
logp	-1.121		Crippen Method
mcvol	153.740	ml/mol	McGowan Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C153285564&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume